Energy gaps in quantum first-order mean-field-like transitions: The problems that quantum annealing cannot solve

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Abstract. - We study first-order quantum phase transitions in models where the mean-field traitment is exact, and the exponentially fast closure of the energy gap with the system size at the transition. We consider exactly solvable ferromagnetic models, and show that they reduce to the Grover problem in a particular limit. We compute the coefficient in the exponential closure of the gap using an instantonic approach, and discuss the (dire) consequences for quantum annealing.

Many important practical problems involve the minimization of a function of discrete variables. Solving such combinatorial problems by temperature annealing is a classical strategy in computer science [1]: the idea is to use thermal fluctuations to avoid trapping the system in local minima, and thereby efficiently visit the whole configuration space. It has been proposed to extend this approach to quantum fluctuations [2]; it is thus of interest to ask whether annealing by tuning down the amplitude of a quantum mechanical kinetic operator such as a transverse magnetic field Γ can outperform the classical approach. In particular, can problems that normally take exponential time be solved in only polynomial time?

Some considerable effort has been devoted to this question in the context of difficult combinatorial problems (see for instance [3]) which have a counterpart in statistical physics where they corresponds to mean-field spin-glass models [4, 5]. However, most of the studies were purely numerical and thus restricted to very small sizes due to the difficulty of simulating quantum mechanics without a quantum computer. In a recent Letter [6] (see also [7]), we argued that with the usual implementation of the quantum annealing it is likely that the most difficult systems undergo a quantum transition of *the first order* as the transverse field is tuned; this is a generic feature for many quantum spin glasses [8]. More recently, a first order transition has indeed been indentified in the phase diagram of one of the most studied random optimization problems, called XORSAT [9]. As we shall see, this implies the failure of quantum annealing for the hardest optimization problems.

The reason why quantum annealing is *not* an efficient strategy for finding the ground state across a first-order transition can be understood from a simple argument. Quantum annealing could *in principle* be more efficient than thermal annealing for certain classes of problems: From the WKB approximation it is well known that a quantum particle tunnels rapidly through very high (in energy) but thin (in distance) energy barriers. Thermal annealing is much better at low, but deep barrier crossing. However, in a first-order transition the two states whose free energies cross are generally *far* from each other in the phase space; quantum tunneling must be inefficient.

To make this argument more precise, and to compute how slow an annealing should be such that the tunelling do happens, one can consider the Landeau-Zener theory of level crossings [2]. During an avoided crossing, the time needed in order to actually reach the ground state is bounded by the inverse of the energy gap Δ between these states. If the total annealing is longer $\tau \gg \Delta^{-2}$, then the adiabtic theorem imply that at each time step, the systems remains in the ground state. Otherwise, the system misses the crossing and is not in the ground state at the end of the computation. A good estimates of the running time of the algoritmh is thus obtain by the minimal energy gap Δ_{min} during the annealing process [2].

We will see that mean-field first-order transitions have

generically an exponentially small gap $\Delta \propto Ne^{-\alpha N}$ where N is the system size. This implies $\tau \gg e^N$, that is to say: quantum annealing is an exponentially slow algorithm for a mean-field system with a first-order transition[1].

The goal of this Letter is to illustrate these features via a complete analytical and detailed numerical analysis for a family of models. We consider the ferromagnetic p-spin model, which reduces to a mean-field ferromagnet for the case $p = 2$ and to the Grover problem when $p \to \infty$. We show how to solve the thermodynamics of these models using standard tools of statistical physics. We perform extensive numerical studies of the gap for the case of p finite and odd. By introducing an ansatz for the dominant instantonic pathways, we show how to compute the coefficient in the exponential decay of the gap.

The simplest quantum ferromagnet. – We consider a Hamiltonian with N Pauli spins σ of the form $\mathcal{H} = \mathcal{H}_z + \Gamma V$ where $\mathcal{H}_z$ is a function of the longitudinal values σ^z of the spins. $\mathcal{H}_z$ is thus diagonal in the σ^z representation. We focus on the ferromagnetic p-spin model:

$$\begin{aligned}\mathcal{H} &= -\frac{1}{N^{p-1}} \sum_{i_1,\dots,i_p} \sigma^z_{i_1} \dots \sigma^z_{i_p} - \Gamma \sum_i \sigma^x_i \qquad (1)\\ &= -\frac{M^p(\vec{\sigma^z})}{N^{p-1}} - \Gamma M^T(\vec{\sigma^x}) = -N\left[m^p(\vec{\sigma^z}) - \Gamma m^T(\vec{\sigma^x})\right]\end{aligned}$$

where we have defined the longitudinal magnetization $M(\vec{\sigma^z}) = \sum_i \sigma^z_i$ and the transverse one $M^T(\vec{\sigma^x}) = \sum_i \sigma^x_i$ and their magnetization by site $m = M/N$ and $m^T = M^T/N$. That sort of models were introduced initially in a spin-glass context in [4, 10]. The ground state of the classical problem, when $\Gamma = 0$, corresponds to all spins aligned in the same direction. Whereas both the *up* and *down* states are valid ground states for even p, the *up* state is the unique ground state for odd p, and we will concentrate on this case for simplicity. The case $p = 2$ is the usual Curie-Weiss model, where the transition is continuous [11, 12]. For $p > 2$ however, both quantum and thermal transitions are discontinuous. Of special interest is the limit $p \to \infty$ where for p odd $m(\{\vec{S}\})^p \to \pm 1$ if $m = \pm 1$, and zero otherwise. It leads to:

$$\mathcal{H} = -N \mathbb{1}\left(\sum_i \sigma^z = N\right) + \Gamma \sum_i \sigma^x \qquad (2)$$

where the function $\mathbb{1}(x)$ is 1 if x is true and zero otherwise. We now specialize to this $p = \infty$ limit.

The $p = \infty$ limit. –

The classical case: $\Gamma = 0$. The $p = \infty$ model is trivial in the limit $\Gamma \to 0$ where there are only two levels with nonzero energies $E = N$ and $E = -N$. The partition sum is thus $Z = 2^N - 2 + 2\cosh \beta N$ so that

$$\begin{aligned} f &= \lim_{N\to\infty} -\frac{1}{\beta N} \log\left(2\cosh \beta N + 2^N - 2\right)\\ &\approx \lim_{N\to\infty} -\frac{1}{\beta N} \log\left(e^{\beta N}\left(1 + e^{N(\log 2 - \beta)}\right)\right)\\ &= \min\left(f_P, f_P\right) \text{ with} \qquad f_F = -1 \text{ and } f_P = -\frac{\log 2}{\beta}\end{aligned}$$

One recognizes a first-order transition at $\beta_c = \log 2$ between two phases that are always locally stable (no spinodal): a ferromagnetic phase that consists of the classical configuration where all spins are up for $\beta > \beta_c$ and a trivial paramagnetic phase at larger temperature.

The extreme quantum case: $\Gamma = \infty$. When Γ is large the classical part of $\mathcal{H}$ can be neglected; we then find, in the σ^x basis, N independent classical spins in a field Γ:

$$f_{QP} = -T \log 2 - T \log\left(\cosh \Gamma/T\right). \qquad (3)$$

The entropy density is given by the logarithm of a binomial in $[-\Gamma N, \Gamma N]$: this is a perfect quantum paramagnet.

The general case. For $\Gamma = 0$ and inverse temperature $\beta < \log 2$ we saw that the classical model is just a model where (almost) all configurations have zero energy. In this case, we thus can ignore the two nonzero levels and we expect the quantum paramagnetic free energy f_{QP} to be valid for all Γ. A simple perturbation computation – given in the next section– shows that this is true in the low-temperature phase as well, when $\beta > \log 2$. The system thus has two distinct phases, the first a quantum paramagnetic and the second a ferromagnetic phase. A first-order transition occurs when the free energies cross so that $f = \min\left(f_{QP}, f_F\right)$. The phase diagram of the model is very simple: For low Γ and T, the free-energy density is that of the classical model in the ferromagnetic phase, while for larger Γ it jumps to the quantum paramagnetic free energy; a first-order transition separates the two different behaviors at the value Γ such that $f_F = f_{QP}$; this happens on the line defined by

$$\Gamma = \frac{1}{\beta} \text{arccosh} \frac{e^\beta}{2} \qquad (4)$$

where the magnetization jumps from 0 to 1 (see Fig. 1).

The zero-temperature behavior can be understood from standard Rayleigh-Schrödinger perturbation theory [13]. Consider the set of eigenvalues E_k and eigenvectors $|k\rangle$ of the unperturbed model, when $\Gamma = 0$. The series for the lowest perturbed eigenvalue $E_{min}(\Gamma)$ reads

$$E_{min}(\Gamma) = E_{min} + \Gamma V_{ii} + \sum_{k \neq min} \frac{\Gamma^2 V_{min\ k} V_{k\ min}}{E_{min} - E_k} + \dots . \qquad (5)$$

Since $V_{ij} \neq 0$ if and only if the two configuration i and j differ by a single spin flip, odd orders do not contribute in Eq. (5). Noting that $\sum_{k\neq n} |V_{nk}|^2$ reduces to a sum over the N levels connected to E_i by a single spin flip, and using the fact that all $E_k = 0$ (except $E_{min} = -N$), succesives terms are easyly computed and one finds, to all (finite) orders (see [6] for a similar computation):

$$E_{min}(\Gamma) = -N - \Gamma^2 + o\left(1\right). \qquad (6)$$

[1] In finite dimensions one expects that nucleation will help. However, optimization problems are not finite dimensional generically.

The expansion can also be performed using now ΓV as a starting point and with $\mathcal{H}_0$ as perturbation. Consider the eigenvalue $-N\Gamma$. In the base $\mid N\rangle$ corresponding to the eigenvalues of ΓV [2], we obtain

$$E(\Gamma) = -N\Gamma + \langle N \mid \mathcal{H}_0 \mid N\rangle + \sum_{k\neq n} \frac{|\langle k \mid \mathcal{H}_0 \mid N\rangle|^2}{-N\Gamma - E_k} + \dots \,. \tag{7}$$

Denoting $a(l)$ the elements of the vector $\mid N\rangle$ in the z basis, the first-order term in this expansion reads $-Na^2(1)$. Since the $a(l)$ are of order $2^{-N/2}$ the first-order shift is tiny. The next term involves a sum over the 2^N-1 levels

$$\sum_{k\neq min} \frac{|a(1)k(1)|^2}{-\Gamma N - E_k} = \sum_{k\neq min} \frac{2^{-N}|k(1)|^2}{-\Gamma N - E_k}\,. \tag{8}$$

The last sum is entropically dominated by the states with $E_k = 0$ and therefore gives a negligible contribution (as one can check term by term). Subsequent terms are treated similarly. This yields the ground-state energy:

$$E_{GS} = -N - \Gamma^2 + o(1) \text{ for } \Gamma < \Gamma_c \tag{9}$$

$$E_{GS} = -\Gamma N + o(1) \text{ for } \Gamma > \Gamma_c \tag{10}$$

$$\text{with} \quad \Gamma_c = 1 + O(1/N). \tag{11}$$

Exponential closure of the gap. Near the transition the treatment must be refined: There is an (avoided) level crossing at $\Gamma_c = 1$ in the large N limit between the paramagnetic and the ferromagnetic ground state. We now compute the behavior of the quantum gap around $\Gamma_c = 1$. We write the Hamiltonian in the σ^x basis:

$$\mathcal{H}_{ij} = \Gamma\varepsilon_i\delta_{i,j} + E_c a_i a_j \tag{12}$$

where $\vec{a}$ is the state corresponding to all spins aligned in the z direction expressed in the x basis. $E_c = -N$ and ε_is are the (binomially distributed) energies due to the quantum interaction. With an appropriate convention for the eigenvectors we can take for a the vector $2^{-N/2}(1,1,1,....1)$. In this basis, on multiplying with an eigenvector $\vec{v}$ of eigenvalue λ, we find

$$0 = (\Gamma\varepsilon_i - \lambda)\, v_i + E_c a_i(\vec{a}.\vec{v}) = v_i + E_c \frac{a_i}{\Gamma\varepsilon_i - \lambda}(\vec{a}.\vec{v})$$

Multiplying again by $\vec{a}$, we find

$$(\vec{a}.\vec{v}) + E_c \sum_i \frac{a_i^2(\vec{a}.\vec{v})}{\Gamma\varepsilon_i - \lambda} = 0 \tag{13}$$

so that

$$\frac{N}{2^N}\sum_i \frac{1}{\Gamma\varepsilon_i - \lambda} = 1\,. \tag{14}$$

The qualitative behavior of the eigenvalues can now be understood graphically: Between each pole in the denominator of Eq. (14) the function passes from $-\infty$ to $+\infty$ passing through unity. All interior roots to the function are thus bracketed by a comb of poles separated by 2Γ. In the small Γ phase this rigorously brackets almost all the eigenvalues near $\lambda = 0$. The exception is the lowest eigenvalue which can split off from the comb, a sign of the phase transition in the large N limit.

In the paramagnetic phase, the lowest eigenvalue is very close to $\lambda = -\Gamma N$. In this case $-\Gamma N - \lambda$ is very small so that we can write $\lambda = -\Gamma N + \eta$. In addition the overwelming majority of eigenvalues ϵ_i are close to zero [3]; Eq. (14) then implies, at the transition when $\Gamma = 1$

$$1 = \frac{N}{2^N}\left[\frac{1}{-N-\lambda} + \frac{2^N-1}{-\lambda}\right] = \frac{N}{2^N}\left[-\frac{1}{\eta} - \frac{2^N-1}{\eta - N}\right],$$

so that finally $\eta^2 = N^2/2^N$ at the critical point and

$$\Delta_{min} = 2N2^{-N/2}\,. \tag{15}$$

The gap closes exponentially fast at the transition. We have an extremely simple model with a first-order mean-field transition and most of the physics discussed in this Letter is already present in this model: difficult problems, such as this one where only one in 2^N configurations has a low energy, manifest themselves by a first-order transition in the quantum annealing path, and consequently by an exponentially small gap.

The reader could at this point argue that we have not shown that *all choices* of the quantum interaction lead to this result; perhaps a more intelligent choice would turn the transition to second order, and make the gap polynomial? We know that for this precise model, this is just impossible. In fact, this model is nothing else than the Grover problem [14], that is: searching for a minimum value in an unsorted database. The best algorithm is known, and it is an exponential one [14]. It is obtained by adjusting the evolution rate of the Hamiltonian in the quantum annealing process so as to keep the evolution adiabatic on each infinitesimal time interval. In doing so, the total running time can be $\tau \propto \Delta^{-1}$ [15], which is still exponential. There is thus no way to avoid the exponential gap in this situation.

Behavior for general p. – We now consider finite value of p and begin by calculating the phase diagram in the static approximation. We then consider closure of the gap using numerical diagonalization and an instantonic calculation which we then compare.

Phase diagram. We shall first use the Suzuki-Trotter formula in order to map onto a classical model with an additional "time" dimension:

$$Z = \sum_{\{\vec{\sigma}\}}\left(e^{-\beta\mathcal{H}_z + \beta\Gamma\sum_i \sigma_i^x}\right) = \lim_{N_s\to\infty} \mathrm{Tr}_{\{\vec{\sigma}\}}\left[e^{-\frac{\beta}{N_s}\mathcal{H}_z} e^{\frac{\beta}{N_s}\Gamma\sum_i \sigma_i^x}\right]^{N_s}$$

$$= \lim_{N_s\to\infty} \sum_{\{\vec{\sigma}\}} \langle\vec{\sigma}| e^{-\sum_{\alpha=1}^{N_s}\frac{\beta}{N_s}\mathcal{H}_z(\alpha)} e^{\sum_{\alpha=1}^{N_s}\frac{\beta}{N_s}\Gamma\sum_i \sigma_i^x(\alpha)} |\vec{\sigma}\rangle\,.$$

[2] Note that in the σ^z basis the ground-state vector $\mid N\rangle$ has elements $\pm 2^{N/2}$.

[3] Systematic corrections to this approximation do not change the result.

We then introduce N closure relations $\mathbb{1} = \sum_{\{\vec{\sigma}\}} |\vec{\sigma}\rangle\langle\vec{\sigma}|$:

$$\begin{aligned} Z &= \sum_{\{\sigma(\vec{\alpha})\}} \prod_{\alpha=1}^{N_s} \langle\sigma(\vec{\alpha})|e^{-\frac{\beta}{N_s}\mathcal{H}_z(\alpha)} e^{\frac{\beta}{N_s}\Gamma\sum_i \sigma_i^x(\alpha)}|\sigma(\vec{\alpha+1})\rangle \\ &= \sum_{\{\sigma(\vec{\alpha})\}} \prod_{\alpha=1}^{N_s} e^{-\frac{\beta}{N_s}\mathcal{H}_z(\alpha)} \prod_{\alpha=1}^{N_s} \langle\sigma(\vec{\alpha})|e^{\frac{\beta}{N_s}\Gamma\sum_i \sigma_i^x(\alpha)}|\sigma(\vec{\alpha+1})\rangle \end{aligned}$$

with the convention that $\sigma(\vec{N_s+1}) = \sigma(\vec{1})$. Applying N_s times the integral representation of the delta function $\int dm\delta(Nm - M(\{\vec{S}\}))f(Nm) = f(M(\{\vec{S}\}))$, one finds:

$$\begin{aligned} Z &= \int \prod_{\alpha=1}^{N_s} dm(\alpha) \prod_{\alpha=1}^{N_s} d\lambda(\alpha) \exp\left(\frac{\beta N}{N_s}\sum_{\alpha=1}^{N_s} m(\alpha)^p\right) \times \\ &\exp\left[\frac{-N}{N_s}\sum_{\alpha=1}^{N_s}\lambda(\alpha)m(\alpha) + N\log \mathrm{Tr}\prod_{\alpha=1}^{N_s} e^{\left[\frac{\beta}{N_s}\Gamma\sigma^x(\alpha)+\frac{\lambda(\alpha)}{N_s}\sigma^z(\alpha)\right]}\right]. \end{aligned}$$

The saddle point condition imposes that $\lambda(\alpha) = \beta p m^{p-1}(\alpha)$. Writing $t = \beta\alpha/N_s$ and performing the limit $N_s \to \infty$ we obtain:

$$Z = \int \mathcal{D}m(t) e^{N\int_0^\beta dt(1-p)m^p(t) + N\log\mathrm{Tr}\, e^{\int_0^\beta dt\Gamma\sigma^x(t)+pm^{p-1}(t)\sigma^z(t)}}. \tag{16}$$

We now use the "static" approximation, which we also check numerically [11, 12], and remove all "time" indices for m to finally obtain:

$$\begin{aligned} Z &= \int dm e^{-\beta N f(\beta,\Gamma,m)} \qquad (17) \\ f(\beta,\Gamma,m) &= (p-1)m^p - \frac{1}{\beta}\log 2\cosh\left(\beta\sqrt{\Gamma^2 + p^2m^{2p-2}}\right). \end{aligned}$$

All thermodynamic quantities can now be computed. For instance, the self-consistent equation for the magnetization m reads (for $p > 2$)

$$m = \left(\frac{\tanh\left(\beta\sqrt{\Gamma^2 + p^2m^{2p-2}}\right)}{\sqrt{\Gamma^2 + p^2m^{2p-2}}}\right) pm^{p-1}. \tag{18}$$

It is easy to check that the former expression leads to first-order (quantum and classical) transitions when its minima cross. In particular, the free energy for $p \to \infty$ is simply $f = -1$ for $m = 1$ and $f = -\frac{1}{\beta}\log 2\cosh(\beta\Gamma)$ otherwise, as we obtained in the first section. The phase diagram of the model is plotted in Fig. 1.

The energy is given by $e = \frac{\partial}{\partial\beta}\beta f$, and thus at low T:

$$\begin{aligned} \mathrm{e}(\beta) &\approx e_{GS} + 2\sqrt{\Gamma^2 + p^2m^{2p-2}}e^{-2\beta\sqrt{\Gamma^2+p^2m^{2p-2}}} \\ \text{with} \quad e_{GS}(\Gamma,m) &= (p-1)m^p - \sqrt{\Gamma^2 + p^2m^{2p-2}}. \end{aligned}$$

In the low-temperature T, the energy of a system with N excited states with an energy gap ΔE is $E = E_{GS} + N\Delta E e^{-\beta\Delta E}$, and this computation thus shows that there

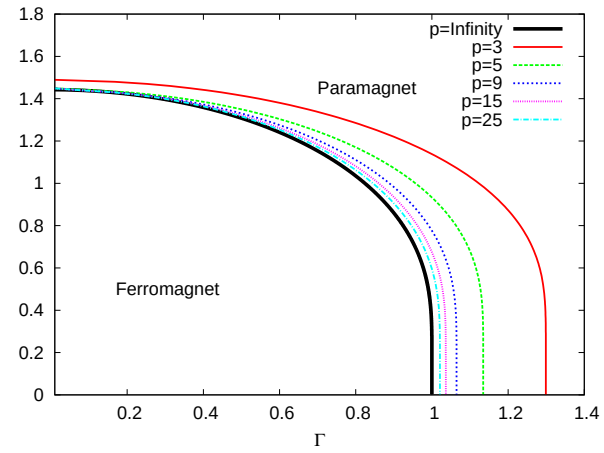

Fig. 1: Phase diagram of the ferromagnetic p-spin ferromagnet for different values of p. A first-order transition separates the ferromagnetic and quantum paramagnetic phases.

are N levels with an energy gap $\Delta E = 2\sqrt{\Gamma^2 + p^2m^{2p-2}}$ where ΔE is discontinuous at the transition.

This is, however, only a crude description of the phenomenology of the low-lying states. If indeed only *one* level is closing at the transition, then we expect the energy to behave as $E = E_{GS} + \Delta E e^{-\beta\Delta E}$, and therefore one needs to compute the $O(1)$ correction to the energy in order to take this into account. The former computation thus misses this behavior and indeed, numerical results show that the first excited state is unique. Worse, we expect the energy gap between the ground state and the excited state to close exponentially fast at the transition, and therefore, in order to be able to investigate this behavior, we should be looking for an exponentially small gap: in that case we thus need to look for exponentially small correction to the free energy! Fortunatly, there is a way to deal with this problem: we now turn to a numerical study of the gap and to the instantonic approach.

Closure of the gap. –

Numerical methods. We use two complementary methods to study the spectrum of the p-spin model for $3 \le p \le 31$. The full matrix representation of the Hamiltonian is a sparse operator of dimension 2^N. For such sparse matrices Laczos methods are particularly useful and can be used to extract extremal eigenvalues from the spectrum for $N \le 21$. We note in particular that that for $N \le 21$ the transition occurs between two states with the maximum possible angular momentum $l = N/2$.

Considerable improvements in efficiency are obtained by realazing that the total angular momentum L^2 commutes with $\mathcal{H}$. Thus the transition occurs in a subspace of dimension $2l+1 = N+1$. In this subspace the Hamiltonian has diagonal elements corresponding to different values of L^z. Standard methods from the theory of angular momentum show that the off-diagonal elements of the matrix in this subspace are only those labeled by $(m_z, m_z \pm 1)$. The

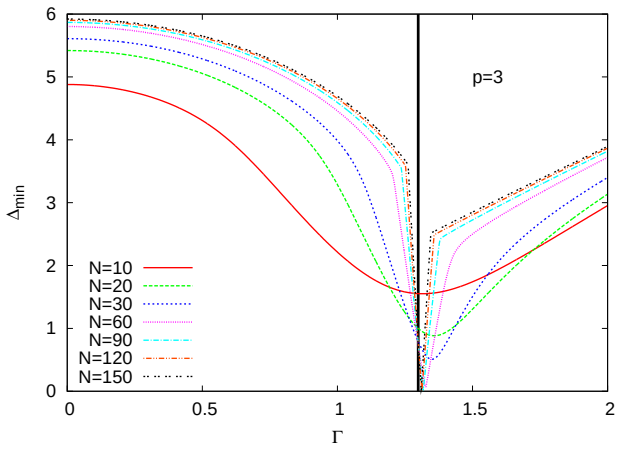

Fig. 2: Numerical computation of the gap versus Γ for $p = 3$ computed using the method described in the text. Very close to the transition at Γ_c (the black vertical line), in a region that shrinks as N increases, the gap is closing exponentially fast.

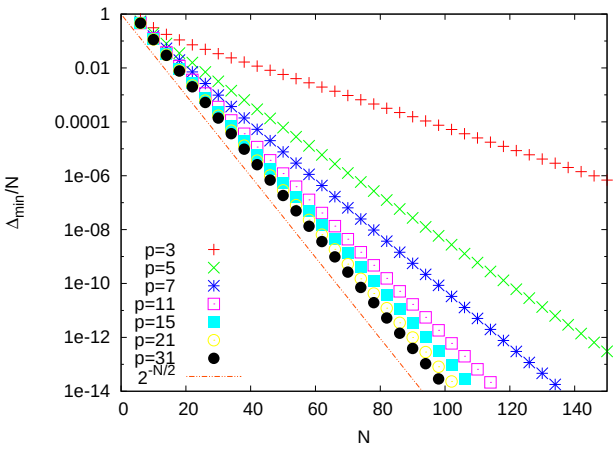

Fig. 3: Minimum Gap versus N from exact diagonalization of the ferromagnetic p-spin model for some values of p on a linear-log scale. One clearly sees that for each p the gap closes exponentially with N, so that $\Delta_{min} \propto N2^{-N\alpha}$.

matrix is symmetric with off-diagonal elements

$$H_{m_z,m_z+1} = \Gamma\sqrt{l(l+1) - m_z(m_z+1)} \qquad (19)$$

The resulting tri-diagonal matrix an be treated with very high efficiency allowing one to study systems of $N \sim 100$ in just a few seconds. The limiting factor in the study of even larger systems is the reduction of the gap to double precision machine accuracy so that floating point round-off errors dominate the results. Fig. 3 shows the dependence of the minimum gap for some values of p. We see that for all $p \geq 3$ the gap closes exponentially in N.

Fig. 2 shows the dependence of the gap Δ as a function function of Γ for $p = 3$ and different N. Δ indeed closes fast at the transition that arises exactly at the critical value predicted analytically. The region where the gap closes is getting narrow as N increases, and one has to be very careful in scanning Γ in order not to miss it: this is an important message for future numerical simulations. Fig. 3 shows the dependence of the minimum value of the gap Δ_{min} as a function of N for some values of p. For all $p \geq 3$, the gap decays exponentially as $\Delta_{min} \propto N2^{-N\alpha}$. The different values of α are given in Table 1. As we expected, the gap closes exponentially fast at the first-order transition point. We want now to show how the coefficient in the exponent can be computed analytically.

The Instantonic approach. It is well known that the tunneling between quantum states can be computed using an instantonic approach [16]. Let us briefly explain how this can be understood via corrections to the saddle-point computation. At the transition, two solutions (the ferromagnetic one $m = m_{eq}$ and the paramagnetic one $m = 0$) have the same free energies $f_m = f_{QP}$. Let us assume now that we are able to find another time-dependent path $m(t)$ —which we shall call instantonic— that spends some time τ_1 in the ferromagnetic state and then jumps to the paramagnetic state where it spends a time τ_2, and that exactly at the transition, one has $\epsilon = e^{-N\beta(f_{inst}-f_{ferro})} = e^{-NG}$ with $G = O(1)$ in the zero-temperature limit. Since we are summing over all periodic paths, one should now take into account all such instantonic paths that jump an even number of times to compute the correction to Eq. (18). Each of these jumps can occur at any time $t \in [0, \beta]$ and the saddle-point computation thus reads, at the transition:

$$\begin{aligned} Z &= 2e^{-\beta F} + 2e^{-\beta F}\left(\frac{\beta^2}{2}\epsilon^2 + \frac{\beta^4}{4!}\epsilon^4 + \frac{\beta^6}{6!} + \dots\right) \\ &= 2\sum_{k \text{ even}} \frac{\beta^k}{k!} e^{-\beta F}\varepsilon^k, \end{aligned} \qquad (20)$$

where the factor $\beta^k/k!$ comes from the counting of all possible paths with k jumps. One then recognizes the series expansion of an effective two level system:

$$Z = \text{Tr } e^{-\beta\mathcal{H}_{eff}}, \text{ with } \mathcal{H}_{eff} = \begin{pmatrix} F & \epsilon \\ \epsilon & F \end{pmatrix}. \qquad (21)$$

Diagonalizing the effective Hamiltonian at $T = 0$ one sees immediately that the gap goes as $\Delta \propto \epsilon = e^{-NG}$: the energy cost of the instanton thus provides the exponent of the gap at the transition.

Computing the Instanton. We can consider various ansätze to compute the optimal instanton, all of them giving lower bounds on the coefficient. The simplest one is just a sharp wall when $m(t)$ jumps abruptly from the value m_Q to m_F. The gap thus reads in this approximation:[4]

$$\Delta = \langle F|Q\rangle^N = e^{N\log\langle F|Q\rangle} \qquad (24)$$

[4] This can be seen in the discrete Suzuki-Trotter formalism where

$$Z = \sum_{\{\sigma(\vec{\alpha})\}} \prod_{\alpha=1}^{N_s} \langle\sigma(\vec{\alpha})|e^{\frac{\beta}{N_s}(\Gamma\sigma^x(\alpha)+h\sigma^z)}|\sigma(\vec{\alpha+1})\rangle\,. \qquad (22)$$

Each term but one can be written in its respective diagonal base (1) or (2) and be computed with the static approach. However, there is

p	Γ_c	m_c	α^{Gap}_{sharp}	α^{Gap}_{tanh}	α^{Gap}_{simu}
3	1.2991	0.8660	0.2075	0.1251	0.126(3)
5	1.1347	0.9682	0.3390	0.2686	0.270(3)
7	1.0874	0.9860	0.3888	0.3335	0.335(3)
9	1.0647	0.9921	0.4150	0.3699	0.370(3)
11	1.0514	0.9959	0.4318	0.3929	0.395(3)
13	1.0426	0.9965	0.4422	0.4105	0.410(3)
15	1.0364	0.9974	0.4502	0.4224	0.421(3)
17	1.0318	0.9980	0.4564	0.4315	0.431(3)
19	1.0282	0.9985	0.4620	0.4387	0.439(3)
21	1.0253	0.9987	0.4648	0.4445	0.445(3)
23	1.0230	0.9990	0.4679	0.4493	0.450(3)
25	1.0211	0.9991	0.4705	0.4534	0.454(3)
31	1.0168	0.9994	0.4763	0.4623	0.462(3)
...	$1+\frac{1}{2p}$	$1-\frac{1}{2p^2}$	$\frac{1}{2}-\frac{\log 2}{p}$	...	$\frac{1}{2}-\frac{1.15...}{p}$
∞	1	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

Table 1: First-order transition in the p-spin ferromagnet at zero temperature: The critical values for the field Γ_c and magnetization m_c are given. The gap at the transition decays exponentially fast as $\Delta \propto N 2^{-N\alpha^{Gap}}$ and we give the numerical results from exact diagonalization α^{Gap}_{simu}, the estimates with the sharp instanton α^{Gap}_{sharp} (an upper bound on the true value) and the soft instanton α^{Gap}_{tanh}: these values are indistinguishable from the numerical ones.

where $\langle F|$ and $\langle Q|$ are the eigenvectors of the matrix

$$\begin{pmatrix} pm^{p-1} & \Gamma \\ \Gamma & -pm^{p-1} \end{pmatrix} \tag{25}$$

Exactly at the transition, this gives an estimates on the gap Δ. In particular for $p \to \infty$, we find that $\Delta \approx N 2^{-N/2}$, as was previously found in the first section. For finite p, however this yields only a crude lower bound on the value of the exponent (see Table 1).

We thus use a *tanh* shape for $m(t)$ and compute numerically the cost, by integrating Eq.(16). We use the width of the *tanh* function as a variational parameter which we vary in order to minimize the estimate of the instanton free energy from which we deduce the gap. The results of this procedure are given in Table 1. When we now compare the numerical data from exact diagonalization with the prediction from the instantonic computation, we observe that there is *no detectable difference within our numerical precision* between the instantonic prediction from the *tanh* shape and the numerical estimation of the coefficient. We have thus obtained Δ from first-principle computations.

Conclusions. – Quantum annealing has been presented as a new way of solving hard optimization problems with complicated and rough configuration spaces. In this paper we have shown that even in systems with trivial energy landscapes quantum annealing can fail (and there is thus no need for more complex phenomena to explain this failure, as for instance in [17]). Already the $p = 3$ ferromagnet exhibits a first-order phase transition with an exponentially closing gap: A scenario which is very pessimistic for the success of the quantum annealing algorithm. We have also shown that the $p = \infty$ limit of the ferromagnetic model is related to the Grover problem. This is a clear indication that these first-order transition carry the signature of the most difficult problems.

Models presented in this Letter allow a complete analytical and numerical treatment. Their disordered counterpart can be studied using the generalized instanton introduced in [6, 7]. It would be interesting to extend this approach to dilute mean-field system and random optimization problems, using the quantum cavity of [9, 12].

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a remaining term of the form

$$\langle \vec{\sigma_1}|e^{\frac{\beta}{N_s}(\Gamma\sigma^x(\alpha)+h\sigma^z)}|\vec{\sigma_2}\rangle = \langle \vec{\sigma_1}|\vec{\sigma_2}\rangle\langle \vec{\sigma_1}|e^{\frac{\beta}{N_s}(\Gamma\sigma^x(\alpha)+h\sigma^z)}|\vec{\sigma_1}\rangle \tag{23}$$